Hexyl acetate

142-92-7 | DTXSID6022006

Model Performance

Model	Data

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.85	0.69	0.86	0.67	0.86	0.78

Model Results

Predicted value: 2.79

Global applicability domain: Inside

Local applicability domain index: 6.99e-01

Confidence level: 8.01e-01

Nearest Neighbors from the Training Set

Image not found
Heptyl acetate
Measured: 3.46
Predicted: 3.40

Image not found
Pentyl acetate
Measured: 2.30
Predicted: 2.27

Image not found
3-Methylbutyl acetate
Measured: 2.25
Predicted: 2.20

Image not found
Isobutyl methacrylate
Measured: 2.66
Predicted: 2.58

Image not found
Hexyl acrylate
Measured: 3.33
Predicted: 3.18